1	Multi-objective optimization of the engine performance and emissions for a
2	hydrogen/gasoline dual-fuel engine equipped with the port water injection
3	system
4	Farhad Salek ¹ , Meisam Babaie * ² , Seyed Vahid Hosseini ¹ , O. Anwar Bég ²
5	¹ Faculty of Mechanical and Mechatronic Engineering, Shahrood University of Technology,
6	Shahrood, Iran
7	² School of Science, Engineering and Environment, University of Salford, Manchester, UK
8	Abstract
9	Hydrogen is one of the most promising options being considered as the fuel of future.
10	However, injection of hydrogen into modern gasoline fueled engines can cause some
11	issues such as power loss. This study, therefore, aims to address this challenge in a
12	simulated hydrogen/gasoline dual-fueled engine by developing a novel and innovative
13	approach without possible side effects such as NOx increment. To achieve this goal, the
14	impacts of water injection and the start of the combustion (SOC) modification in a
15	gasoline/hydrogen duel fueled engine have been rigorously investigated. In current
16	methodology, an engine is simulated using AVL software and the model is validated
17	against the experimental data. The Latin Hypercube design experiment method was
18	employed to determine the design points in 3-dimensional space. Due to the existing
19	trade-off between NOx and BMEP, multi-objective optimization using genetic algorithm
20	(GA) was implemented to determine the optimum values of water injection and SOC in
21	various hydrogen energy shares and the effects of optimum design parameters on the
22	main engine performance and emission parameters were investigated. The results
23	showed that the proposed solution could recover the brake mean effective pressure
24	(BMEP) and in some hydrogen energy shares even increase it above the level of single

fueled gasoline engine with the added benefit of there being no increase in NOx compared to the original level. Furthermore, other emissions and engine performance parameters are improved including the engine equivalent Brake specific fuel consumption (BSFC) which was shown to increased up to 4.61%.

5 Keywords: Hydrogen/gasoline dual fueled engines; Latin Hypercube design experiment
6 method; Multi-objective optimization; BMEP; BSFC.

7 1. Introduction

8 Emission reduction from internal combustion (IC) engines is a major challenge for the transport sector (1). To overcome this issue, the automotive industry has implemented a 9 variety of different technological solutions for emission reduction and a concerted shift 10 11 towards electrification of the powertrain system (2). Recently, different types of hybrid and electric vehicles such as Hybrid Electric Vehicles (HEVs), Battery Electric vehicles 12 (BEVs) and Fuel Cell Hybrid Electric Vehicles (FCHEVs) have been introduced with 13 the aim of reducing emissions. However, there are still numerous challenges facing 14 electric vehicles including the low energy density of Lithium-ions, heavy battery weight 15 16 and high capital cost as well as the limitation of Lithium resources and environmental 17 concerns of mining (3). Furthermore, phasing-out the IC engines could take a decade or so in Europe while it would be slower in developing countries. In light of this, evidently, 18 19 IC engines have a long life ahead even for road transport. Consequently, electrification 20 cannot be viewed as the only solution for resolving the emissions of modern transportation systems. Other options such as dual fuel systems could be considered for 21 22 conventional IC engines in which the injection of an auxiliary fuel can reduce the fuel 23 consumption and improve the engine performance by emitting less pollutions (4, 5). Recently, hydrogen has been proposed as the green fuel of the future (6, 7). Hydrogen 24

oxidation will not generate any chemical pollutant (8), and is therefore a viable 1 alternative for fossil fuels in vehicles. However, there are some conceptual issues for 2 3 running IC engines with 100% hydrogen and major modifications are needed in the engine. Instead, for an intermediate solution, hydrogen can be employed as an auxiliary 4 fuel in vehicles with the goal of reduction in fuel consumption and emissions(9, 10). For 5 6 instance, in a recent study by Zhou et al. (11), it was shown that adding hydrogen to the 7 vehicle fuel can lead to reduction of fuel consumption price and the emission production 8 rate.

9 As reported by different researchers (12-14, 15, 16, 17), engine performance is significantly affected by hydrogen injection due to its high flammability and heating 10 11 value. Geca and Litak (18) measured engine peak pressure fluctuations by injecting hydrogen as the secondary fuel for various energy shares of hydrogen ranging from 5% 12 13 to 20%. The in-cylinder peak pressure fluctuation affected the dynamical combustion 14 process due to the existence of hydrogen content in the combustion chamber (17). When the air-fuel ratio is fixed, a reduction of engine thermal efficiency, engine power and 15 NOx emission with hydrogen injection were concluded (11, 17). As reported by Magryta 16 17 (15) and Ji (19), injecting hydrogen by various *energy shares* into the engine results in a decrease in engine thermal efficiency, power output and NOx emissions. The reduction 18 19 in engine power could be avoided when changing the air to fuel ratio by adding the 20 hydrogen as an extra fuel as reported by Kim et al. (12). According to their experimental results, adding hydrogen can improve the engine thermal efficiency, however, the 21 increase in NOx was also reported by hydrogen injection in this study due to the increase 22 23 in combustion temperature.

Water injection and ignition timing modification can overcome the challenge of power
reduction by hydrogen injection and successfully reduce NOx emission (18, 20-24). Start

of combustion (or spark timing) is an important parameter which can affect the 1 performance of the hydrogen-gasoline fueled engines (18, 21, 25, 26). The engine 2 3 ignition timing should be modified when hydrogen is to be injected into the engine since it significantly affects the engine emissions and thermal efficiency (27, 28). Water 4 injection is also a solution for NOx reduction as recommended by Chintala et al. (29) in 5 6 a study for simultaneous water and hydrogen injection into the engine. Hydrogen and 7 oxygen mixture were injected into the engine at various volumetric flow rates and water 8 was added into the engine intake manifold with the goal of NOx reduction in this study. 9 Based on their results, it was found that water injection reduced the engine NOx emission by approximately 60%; however, the HC was increased. Another similar study was 10 accomplished by Dhyani et al (28) on controlling the NOx generation rate and backfire 11 12 in a spark ignition engine. As it is reported by them, injection of water into the engine resulted in significant reduction of engine NOx production rate, and it is recommended 13 14 an effective way for controlling the backfire during the combustion. The impacts of coinjection of water and hydrogen on performance and emission production of a spark 15 ignition engine fueled by natural gas was studied by Wang et al (22). In this research, the 16 engine was modeled by a 2D engine modelling software. The results showed that 17 injection of water reduce the engine power and NOx emissions. Furthermore, it was also 18 reported that engine HC and CO production rates were increased due to the reduction of 19 20 the combustion chamber temperature.

Numerical analysis of engine performance is a common practice in modern automotive engineering. For example, a numerical 2-D study was employed by Ji *et al.* (27) and Magryta *et al.* (15) and other researchers (30-33) for simulating hydrogen addition into the engine. It was shown in both studies that the results from numerical simulation in AVL simulation software has a strong agreement with experimental data. Furthermore,

the negative impacts of adding hydrogen on engine thermal and volumetric efficiencies 1 were confirmed by Magryta et al. (15). Furthermore, in many relevant studies, design of 2 3 experiment methods such as response surface methodology have been used to investigated the effects of adding different fuels on engine performance and emissions 4 (34-36). Employment of design of experiment methods in experiments and numerical 5 analysis of engines results in figuring out the mathematical relation between design (or 6 7 functional) parameters and engine various outputs. In addition, the regression analysis can be employed to define an equation for each response in DOE methods which can be 8 9 used in optimization process (34).

10 As discussed above, the injection of hydrogen into the engine at *fixed air to fuel ratio* will incur some negative effects on the engine performance such as reduction of thermal 11 efficiency and power (15, 27). Injection of water and modification of the SOC angle are 12 13 two efficient ways for increasing the power (18, 21, 23, 24, 27, 29, 37), so they can be 14 employed for hydrogen-gasoline fueled engines. However, the potential of water injection and SOC in improving the power loss resulted from hydrogen injection as well 15 as the engine thermal efficiency has not been investigated. In this study, the *novel idea* 16 17 of water injection and tuning the SOC are proposed for a hydrogen-gasoline fueled engine in which the hydrogen is injected with various energy shares. To overcome the 18 19 challenge of power loss and realized the environmental benefits of hydrogen injection, 20 the aim is to optimize the engine *BMEP* and *NOx* based on water injection rate and start of combustion (SOC) at different hydrogen energy shares. To achieve this aim, the engine 21 22 has been simulated with AVL BOOST software and validated against the experimental 23 data. The Latin Hypercube design of experiment method was employed to determine the design points in 3D space. Three design variables have been considered in this study: H_2 24 25 energy share, water injection ratio (WIR) and start of combustion (SOC) in the model

with two objective functions, i.e. BMEP and NOx. A regression analysis has been utilized 1 to provide the equations required in the optimization process for the objective functions. 2 3 To establish the optimum values of water injection and SOC angle for each hydrogen energy share, multi-objective optimization using Genetic algorithm (GA) is deployed. 4 Next, the engine performance is evaluated at the optimum point for the engine rated 5 6 condition (6000 RPM). To demonstrate the effectiveness of the proposed method, the 7 optimized engine has further been compared with hydrogen-gasoline fueled engine and original single gasoline fueled engine for several engine performance and emission 8 9 criteria.

10 2. Methodology

11 2.1 Experimental set-up

Figure 1 shows the engine test bed and the related eddy current dynamometer. The 12 13 schematic diagram of engine test bed is also presented in **Figure 2**. The test bed was developed for a KIA Cerato engine which is the case study of this research. The KIA 14 Cerato engine specifications are presented in **Table 1**. Initially, the engine was tested at 15 16 various operating conditions to collect the experimental data used for validating the 17 model. The engine tests were performed in steady state condition at rated RPM. The main engine functional parameters such as fuel consumption rate (for calculation of BSFC), 18 19 engine torque and NOx emission were measured and used for validation of the 20 mathematical model in this research.

At engine test room, the Schenck 190 kW dynamometer was employed to run the engine for collecting the data at different RPMs. During the experiments, the engine functional parameters were recorded and used for validation of engine mathematical model which is explained in following sections. The engine test standard code and laboratory testing

- 1 and calibration standard code are ISO 1585 and ISO 17025, respectively. Moreover, the
- 2 uncertainty analysis of testing instruments is presented in **Table 2**.
- 3

Table.1 Specifications of KIA Cerato engine

Parameter	Unit	Value
Bore	mm	86
Stroke	mm	86
Connecting rod length	mm	143.5
Number of Cylinders		4
Maximum Power	kW	92
Maximum RPM	RPM	7000
Rated RPM	RPM	6000
Compression Ratio		10.5



(a)





Fig.1 The KIA Cerato engine test bed





Parameter	Unit	Measuring equipment	Nominal	Uncertainty	Relative
			value range		uncertainty [%]
Air temperature	°C	Dina Engine Connect	0-100	<u>+</u> 2	2
Air pressure	kPa	(38)	0-100	<u>+</u> 1	1
Relative	%		5-95	<u>+</u> 2.5	2.63
humidity					
Fuel temperature	°C		0-100	<u>+</u> 0.2	0.2
Engine speed	RPM	Schenck 190 kW	100-7000	<u>+</u> 4	5.71
Engine torque	Nm	Dynamometer (38)	0-250	<u>+</u> 0.95	0.38
Engine power	kW		0-190	<u>+</u> 1.2	0.63
NOx	ppm	Testo 350	0-4000	<u>+</u> 10	0.25
Engine fuel	kg/h	Dina Fuel Mass Flow	1-50	<u>+</u> 0.25	0.5
consumption		Meter (38)			

3 **2.2 Engine mathematical model**

For developing the mathematical model of the KIA Cerato engine, AVL BOOST
software was used. AVL BOOST is a 2D simulation software which performs highly
accurate numerical analysis of the engines. It can deliver an advanced analysis for
detailed prediction of engine performance and tailpipe emissions and it has been widely
used by different researchers and automotive industries.

9 The block diagram of the model developed in AVL boost software are visualized in
10 Figure 3. As shown, this engine configuration has 6 injectors (I1-I6). Injector 5 (I5) and
11 6 (I6) are employed for injection of hydrogen and water, respectively. After designing

Table.2 Uncertainties of measuring instruments

the block diagram of the proposed engine in the software, appropriate input parameters and mathematical models should be assigned to the model for enabling the software to provide the accurate output data using a set of complex algorithms. Formula Interpreter (FI1) block is used to calculate specific parameters such as the equivalent BSFC which are obtained by solving the external equations. Furthermore, water was injected into engine using single port injector as shown in Figure 3.



Fig.3 Block diagram of engine model in AVL BOOST software

8

1 **2.2.1** Combustion model

The Vibe two-zone combustion model (15) is employed for mathematical modeling of the combustion process. This model is widely used in single and dual fuel engine systems for engine and emission analysis (39-46). The combustion chamber is divided into two zones, namely the *burned* and *unburned* zones. Therefore, this model can provide a meaningful prediction of unburnt hydrocarbon in unburned zones as well as the combustion. By applying first law of thermodynamic for each region the following equations are achieved (44):

9
$$\frac{dm_b u_b}{d\alpha} = -P_c \frac{dV_b}{d\alpha} + \frac{dQ_f}{d\alpha} - \sum \frac{dQ_{wb}}{d\alpha} + h_u \frac{dm_b}{d\alpha} - h_{BB,b} \frac{dm_{BB,b}}{d\alpha}$$
(1)

10
$$\frac{dm_u u_u}{d\alpha} = -P_c \frac{dV_u}{d\alpha} - \sum \frac{dQ_{wu}}{d\alpha} - h_u \frac{dm_B}{d\alpha} - h_{BB,u} \frac{dm_{BB,u}}{d\alpha}$$
(2)

11 Where dm_u , $P_c \frac{dV_b}{d\alpha}$, $\frac{dQ_f}{d\alpha}$, $\frac{dQ_w}{d\alpha}$, $h_u \frac{dm_b}{d\alpha}$ and $h_{BB,b} \frac{dm_{BB,b}}{d\alpha}$ terms are variation of in-cylinder 12 internal energy, piston work, fuel input energy, wall heat losses, enthalpy flow from 13 unburnt to burnt zone and blow by enthalpy, respectively. For volume changes of each 14 zone, the equations can be expressed as follow (44):

15
$$\frac{dV}{d\alpha} = \frac{dV_b}{d\alpha} + \frac{dV_u}{d\alpha}$$
 (3)

$$16 \quad V = V_b + V_u \tag{4}$$

In the Vibe two-zone model, the fuel mass burned fraction (*x*) during combustion is
expressed as below (33, 44):

19
$$x = 1 - \exp\left[-a\left(\frac{\alpha - SOC}{BDUR}\right)^{m+1}\right]$$
(5)

1 Here, SOC, BDUR, \propto , m and a are parameters representing the start of the combustion, 2 burn duration, crankshaft angle, Vibe shape and Vibe parameter, consecutively. Vibe shape parameter indicates the position of the brunt for the combustion position. By 3 employing such a combustion model with less complexity, large amount of time can be 4 5 saved in simulation specially when the optimization is involved. However, the model should be precisely validated prior to any analysis. Vibe two-zone model has been used 6 in previous related studies in the field (15, 47-49) and selected for this study as well, 7 8 while a detailed validation process was performed.

9 2.2.2 Heat transfer model

The Woschni 1978 heat transfer model was used for modelling of the heat transfer between gas and cylinder walls (33, 44, 50-52). This model accounts for the increase in the gas velocity in the cylinder during combustion and is superior to earlier models which generally assume a constant characteristic gas velocity equal to the mean piston speed. In Woschni 1978 in-cylinder heat transfer model, the heat transfer to the walls of the combustion chamber, i.e. the cylinder head, the piston, and the cylinder liner, is calculated from:

$$17 \quad Q_{wi} = A_i \alpha_w (T_c - T_{wi}) \tag{6}$$

18 Where Q_{wi} , A_i , α_w , T_c and T_{wi} are wall heat flow, surface area, heat transfer 19 coefficient, gas temperature in the cylinder and wall temperature, respectively. The α_w 20 for the high-pressure cycle in Woschni 1978 model is summarized as follows (53):

21
$$\alpha_w = 130D^{-0.2}p_c^{0.8}T_c^{-0.53} \left[C_1 c_m + C_2 \frac{V_D T_{c,1}}{p_{c,1} V_{c,1}} (p_c - p_{c,0}) \right]^{0.8}$$
 (7)

22
$$C_1 = 2.28 + 0.308 \frac{c_u}{c_m}$$
 (8)

D, c_u, c_m, V_D, p_{c,0}, T_{c,1} and p_{c,1} are cylinder bore, circumferential velocity, mean
piston speed, displacement per cylinder, cylinder pressure of the motored engine,
temperature in the cylinder at intake valve closing (IVC) and pressure in the cylinder at
IVC, consecutively. C₂ equals to 0.00622 in this study because the engine used in this
paper equipped with in-direct injection system. The Woschni 1978 model uses equation
provided below for heat transfer coefficient in gas exchange process:

7
$$\alpha_w = 130 D^{-0.2} p_c^{0.8} T_c^{-0.53} [C_3 c_m]^{0.8}$$
 (9)

$$8 \quad C_3 = 6.18 + 0.417 \frac{c_u}{c_m} \tag{10}$$

9 **2.2.3 Emission model**

The Pattas and Hafner equation (33) combined with Zeldovich mechanism are employed
for mathematical modeling of NOx formation rate in AVL BOOST as provided below
(33):

13
$$r_{NO} = C_{PPM} C_{KM}(2,0) (1 - a_{NO}^2) \left[\frac{r_1}{1 + a_{NO}AK_2} + \frac{r_4}{1 + AK_4} \right]$$
 (11)

$$14 a_{NO} = \frac{C_{NO.act}}{C_{NO.equ}} \frac{1}{C_{KM}} (12)$$

15
$$AK_2 = \frac{r_1}{r_2 + r_3}$$
 (13)

16
$$AK_4 = \frac{r_4}{r_5 + r_6}$$
 (14)

Where C_{PPM} , C_{KM} , C_i and r_{NO} are post processing multiplier, kinetic multiplier, molar concentration and reaction rate of NOx, respectively. The equation provided by Onorati et al. (33) is used for modeling of CO formation:

1
$$r_{CO} = C_{cte}(r_1 - r_2) [1 - a_{CO}]$$
 (15)

$$a_{CO} = \frac{c_{CO.act}}{c_{CO.equ}} \tag{16}$$

where r_{NO} and C_i are CO reaction rate and molar concentration, consecutively. Moreover, the complex phenomenological model for prediction of HC formation developed by AVL BOOST is employed for modeling of unburned hydrocarbons (HC) (33).

7 2.2.4 Fueling system parameters

8 In this study hydrogen has been injected to engine as secondary fuel, the lower heating
9 value (LHV) of which is higher than that of gasoline fuel. Therefore, the equivalent
10 BSFC has been computed using Eqn. (17) as presented below:

11
$$BSFC_{eqv} = \frac{\dot{m}_{gasoline} + \dot{m}_{H2} \frac{LHV_{H2}}{LHV_{gasoline}}}{\dot{W}_{engine}}$$
(17)

Here $\dot{m}_{gasoline}$, \dot{m}_{H2} and \dot{W}_{engine} are the gasoline mass flow rate, hydrogen mass flow rate and engine power output parameters, respectively.

The hydrogen is injected into the engine at different energy shares. The hydrogen energy share shows the fraction of energy supplied by hydrogen instead of using gasoline fuel. The mass flow rates of hydrogen and gasoline fuels in various hydrogen energy shares are presented in **Table 3**. The *mass flow rate of hydrogen injection* in various engine conditions can be expressed as:

$$19 \quad \dot{m}_{H2} = \dot{m}_{total\ fuel}\ mf_{H2} \frac{LHV_{gasoline}}{LHV_{H2}} \tag{18}$$

1	In Eqn. (18) $\dot{m}_{total fuel}$ and mf_{H2} are the total mass flow rate of fuel and hydrogen
2	energy share, respectively. In addition, water is injected into engine at different engine
3	speeds with different water-to-fuel ratios:

$$4 \quad \dot{m}_{water} = \dot{m}_{total\ fuel} WIR \tag{19}$$

5 Where *WIR* and *m_{water}* designate the water-to-total fuel ratio and water mass flow rate,
6 respectively. The water injection ratio is calculated using Eqn. (20):

7
$$WIR = \dot{m}_{water} / \dot{m}_{total fuel}$$
 (20)

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- 9

Table.3 Specifications of KIA Cerato engine

Hydrogen energy share	Gasoline mass flow rate	Hydrogen mass flow rate
	[g/s]	[g/s]
0	8.47	0
0.05	8.058	0.149
0.1	7.649	0.288
0.2	6.866	0.537
0.3	6.123	0.748

10

11 **2.3 Design of experiments analysis**

Having an increasing number of parameters, the optimization process is going to be complex for this study. By employing the Design of Experiment (DoE) Methods, an optimized number of parameters can be generated in design space to run an efficient

1 optimization process. In order to perform a parametric analysis for investigating the 2 effects of injecting hydrogen and water into the engine, the Latin Hypercube DOE (design of experiments) method was used (54-57). In Latin Hypercube DOE method, 3 random design points are generated in a multi-dimensional distribution. In this study, 4 5 hydrogen energy share, water injection ratio and SOC were chosen as the design parameters in DOE method. The distribution of design points in the Latin Hypercube is 6 7 shown in Figure 4. Each axis of Latin hypercube in Figure 4, belongs to the one of the design parameters defined for this study and the maximum and minimum values for each 8 9 of the design parameters are also presented in Table 4.





11 Fig.4 The sampling space and the design points in Latin Hypercube DOE method

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- 14

Table.4 Maximum and minimum values of each design parameter

Parameter	Unit	Minimum value	Maximum value
H2 energy share	-	0	0.3
Water injection ratio	_	0	0.3
		, i i i i i i i i i i i i i i i i i i i	010
SOC	Degree	-20	0
			5

2

There are 200 design points in sampling space of the Latin Hypercube. Therefore, each
response will be calculated for all 200 points in the sampling space for this study.
Following this, the regression will be employed to obtain relationships between
responses and design parameters which lead to the *optimization* phase.

7 2.4 Multi-objective optimization

As mentioned in previous section, the relation between each of the responses and design 8 9 parameters were obtained by using regression analysis. The equation obtained from 10 regression analysis are used for multi-objective optimization using genetic algorithm (GA) method (58, 59). The optimization criteria are provided in Table 5. There is a trade-11 of between the selected two objective functions (BMEP and NOx_{MFR}) for selected design 12 parameters (hydrogen energy share, water injection ratio and SOC), that's why multi-13 14 objective optimization was performed using MATLAB software. The pareto front 15 diagrams showing the optimum point for each hydrogen energy share were obtained 16 during optimization. Then, the ideal point in each pareto front diagram indicating the 17 optimum point for each hydrogen energy share was identified.

18

Table.5 The optimization criteria

Objective	Criterion	Minimum value	Maximum value
BMEP [bar]	Max	8.84	10.04
NO x _{MFR} [kg/s]	Min	25e-6	55e-6

2

The principal targets of multi-objective optimization are *maximizing BMEP* (minimizing
-BMEP) and *minimizing NOx* emissions. Figure 5 presents the procedure in which the
experiments, mathematical modelling and optimization process were performed





Fig.5 The flow chart of experiments and optimization process in this study

2

4 **3. Validation**

For validation of the AVL model, the BSFC, engine torque output and NOx have been
compared with experimental results. The experiments were conducted precisely using a
specialized testbed and the required results were extracted for validation. The results of
the comparison are illustrated in **Table 6**. Inspection of this table demonstrates that the

model is in good agreement with the experimental data for different conditions. As can
be seen, the errors are higher in low RPMs compared to high RPMs as the result of the
less stability of the engine at lower RPMs. Furthermore, the maximum error arising from
the comparison of data between the experiments and the AVL model is below 8%.
Therefore, the validity of the model is confirmed, and it is applied with justifiable
confidence in the rest of this investigation.

Engine	Engine tor	Engine torque [Nm]			Engine BSFC			x production rat	te
speed				[g	/kWh]			[ppm]	
(RPM)	AVL model	Experiment	Error	AVL	Experiment	Error	AVL	Experiment	Error
			[%]	model		[%]	model		[%]
1000	137.1	148.1	7.434	299	306.5	2.44	478	444	7.65
2000	152.8	161.9	5.627	275.1	294.9	6.721	804	843	4.62
4000	185.4	191.7	3.312	284.7	273.3	4.157	672	650	3.38
6000	151.9	153.1	0.7838	319.9	319.8	0.024	558	540	3.3
6500	136.9	140.2	2.375	337.3	342	1.387	439	456	3.72
7000	123.9	129.8	4.569	352.2	358	1.611	413	402	2.73

Table.6 Comparison of engine torque, BSFC and NOx production rate of AVL model with experimental tests in different RPMs

1 **4. Result and discussion**

2 **4.1 Regression and variance analysis**

The regression analysis was performed to define the relationship between the objective functions (BMEP and NOx) and design parameters (H2 energy share, WIR and SOC) for the multi-objective genetic algorithm (GA) optimization. Two selected objective functions (called "Responses") are presented in **Table 7** and are defined based on the design parameters elucidated in Eqn. (21) as follows:

8 Response =
$$cte + a.SOC + b.H2_{ES} + c.WIR + d.SOC.H2_{ES} + e.SOC.WIR +$$

9
$$f.H2_{ES}.WIR + g.SOC^2 + h.H2_{ES}^2 + i.WIR^2$$
 (21)

10 The constant parameters and multipliers of Eqn. (21) are presented in **Table 7** for each 11 of the objective functions (Responses) at the rated condition (6000 RPM). The fitting 12 goodness analysis for each Response (BMEP and NOx) has also been performed and the 13 results are provided in **Table 8**. As shown, the *maximum error of regression fitting* is 14 below 1% which is a strong verification of the high precision achieved with the current 15 mathematical model.

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- 17
- 18
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- 20

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Table.7 The regression constant parameters and multipliers

Responses	cte	a	b	с	d	е	f	g	h	i
BMEP	8.971	-0.109	-2.412	3.653	-0.0096	-0.0067	4.469	-0.0038	0.0896	-5.699
Indicated Efficiency (IE)	0.339	-0.003	0.144	-0.25	-0.001	0.0009	-0.211	-0.0001	0.113	0.099
PCT	2501.52	-5.35	-99.84	82.22	-3.48	1.97	468.01	0.214	49.36	-789.41
NOx production	3.581e-5	-3.409e-6	-9.141e-5	2.883e-	4.503e-6	-2.313e-6	0.0003	2.769e-8	2.785e-5	0.00035
				5						
				5						
HC production	3.566e-5	-7.876e-7	-2.590e-5	3.17e-5	3.914e-7	-6.864e-7	-1.238e-6	1.459e-9	2.152e-6	-3.703e-6
CO production	0.006	2.828e-5	-0.0005	-0.0032	-2.763e-5	-6.519e-6	-0.0018	5.504e-7	-0.0049	0.00066

Table.8	The	fitness	analysis	of re	gression
			m	~	5

Responses	P-value	R ²
BMEP	<0.0001	0.99
IE	<0.0001	0.99
РСТ	<0.0001	0.99
NOx production	<0.0001	0.99
HC production	<0.0001	0.99
CO production	<0.0001	0.99

4.2 Multi-objective optimization

The equations developed by regression analysis in the previous section were used in the optimization process. As elaborated in the literature review, hydrogen injection will result in power reduction in engines (15, 19). On the other hand, any attempt to compensate this power reduction, would increase the NOx production (12), and a trade-off, therefore, exists. In accordance with the constraints, BMEP and NOx production rate have been considered as the objective functions for the optimization process. The optimization is performed to determine as accurately as possible, the optimum values of WIR, SOC for each hydrogen energy shares.

Figure 6 presents the Pareto frontier for one of the hydrogen energy shares. As shown,
a clear trade-off between 2 objective functions are observed. The nearest point (optimum
design point) to the ideal point is also identified. The behaviors for other energy shares
were the same and all of the optimum design points (nearest point to ideal point) for each
hydrogen shares are summarized in Table 9.

Based on the results provided in **Table 9**, water should be injected at the maximum rate
to optimize the engine while the optimum values of SOC angle vary in the range between
-6.23 and -2.65 for various hydrogen energy shares.



Fig.6 The Pareto optimal frontier for the H2 energy share of 0.05

Hydrogen energy share	Optimized values						
	Water injection ratio	Start of combustion (SOC)					
		[deg]					
0.05	0.3	-5.9					
0.1	0.3	-5.19					
0.2	0.3	-6.23					
0.3	0.3	-2.65					

2 **Table.9** The optimum design point specifications for various hydrogen energy shares

3

4 **4.2** Parametric analysis and comparison

5 To further develop the analysis, *four optimum designed points* obtained in the previous 6 section were used in the model to study the engine performance in different scenarios. 7 The comparison was made to investigate the benefits of optimized water injection and 8 SOC on various engine performance parameters. The results of optimized co-injection 9 were compared to the single fueled gasoline engine (same engine without hydrogen and 10 water injection) and with the hydrogen dual fueled engine without any water injection 11 and SOC modification.

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2 **Fig.7** The engine BMEP for various hydrogen energy shares with different fueling

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modes

Figure 7 shows the BMEP trend by hydrogen injection for various hydrogen energy 4 shares. As can be seen, injection of hydrogen to the engine reduces the engine BMEP 5 6 compared to the original engine operating purely on gasoline fuel. The reduction in BMEP is between 1.36% to 7.33% with the highest reduction corresponding to the 7 highest hydrogen injection which is mainly attributable to the reduction of engine 8 9 volumetric efficiency, as also reported by Magryta et al. (15). However, the optimized injection of water with SOC modification clearly exerts a positive effect and recovers the 10 engine BMEP; additionally, an increase of 8.8% in BMEP is observed at 5% hydrogen 11 energy share. Therefore, the SOC modification with optimized injection of water has 12 been shown to not only completely compensate the BMEP drop caused by hydrogen 13 14 injection into the engine, but to achieve a supplementary boost in BMEP value.



Fig.8 The engine brake thermal efficiency for various hydrogen energy shares with

different fuel modes





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Fig.9 The net rate of heat release at various crank angles at hydrogen energy share of

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The variation of engine brake thermal efficiency at various hydrogen shares is shown in 1 Figure 8. According to the results, injection of hydrogen without any modification 2 results in reduction of engine brake thermal efficiency between 0.3% and 1.2% for 3 various hydrogen energy shares. On the other hand, by injection of water and 4 modification of SOC with optimum values, the engine brake thermal efficiency is 5 distinctly improved when compared to the single fueled engine for different hydrogen 6 7 energy shares. The impact of optimization of SOC and water injection rate on the net rate of heat release at hydrogen energy share of 0.2 is presented in Figure 9. As can be seen, 8 9 the peak value of heat release is slightly higher for optimal case, and the it is shifted to the right. This increment of rate of heat release resulted by optimal injection of water and 10 modification of SOC has reflected on increase of engine BMEP and brake thermal 11 12 efficiency as presented in Figures 7 and 8.

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15 **Fig.10** The engine equivalent BSFC at various hydrogen energy shares with different

fuel modes

1 The effects of hydrogen injection on BSFC for different fueling modes are presented in **Figure 10**. The engine equivalent BSFC is enhanced via injection of hydrogen at various 2 hydrogen shares up to 4.61% in comparison to the condition where engine is fueled by 3 gasoline due to the engine power reduction (as a result of the decrease in BMEP). 4 However, by simultaneous optimization of the water injection and SOC, the engine 5 equivalent BSFC is decreased between 1.23% and 3% compared to the original condition 6 7 for different H₂ energy shares. This confirms the positive effect of the adopted optimization approach on fuel consumption for hydrogen addition into the fuel. 8



Fig.11 The engine CO production rate at various hydrogen energy shares with different

fuel modes

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Fig.12 The engine HC production rate at various hydrogen energy shares for different
fuel modes

4 The effects of H₂ injection on CO and HC emissions are presented in Figures 11 and 12. As indicated, the CO production decreases continuously by injection of hydrogen up to 5 8.8%, whereas optimized co-injection of water results in a significant reduction of about 6 7 25% compared to the original condition (due to the improvement of combustion performance by injection of water and modification of SOC angle with optimum values). 8 9 However, the trend for HC is not the same. While hydrogen injection caused a continuous reduction in HC emissions between 2.4% to 19.5% compared to original condition, 10 11 optimized injection produces an increase in engine HC production from the hydrogen 12 shares of between 5%-20%. Since Hydrogen is not a hydrocarbon fuel and the hydrogen molecules do not contain any carbon, increment of hydrogen mass fractions in the fuel 13 results in reduction of HC production rate. On the other hand, injection of water into the 14 15 engine results in reduction of the in-cylinder mixture temperature. This reduction in temperature leads to increase of unburnt local zones inside the cylinder resulting in 16

increase of HC production rate. Increase in HC production rate could be caused by the *moderate increase of unburnt zones* in the combustion chamber induced by virtue of an
increase of water content in the combustion chamber. Only when the hydrogen share
reaches 30% does the engine HC level drop below the gasoline fueled engine.



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6 Fig.13 The engine NOx production rate at various hydrogen energy shares for different





Fig.14 The cylinder peak temperature at various hydrogen energy shares for different

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fuel modes

3 The engine NOx emission rate at various hydrogen shares for different fueling modes are displayed in Figure 13. NOx production rate is decreased by hydrogen injection for both 4 optimized and unoptimized scenarios. However, optimized co-injection of water and 5 6 SOC modification influence engine performance more positively in terms of NOx 7 reduction and a significant NOx reduction (up to nearly 59%) is achieved. The reduction in NOx could be relevant to *in-cylinder temperature decrease* when water is injected as 8 9 shown in Figure 14. NOx reduction trend was reported by Ji et al. (19) in the literature. The other reason is the reduction of engine volumetric efficiency which results in engine 10 torque and cylinder pressure reduction by injection of hydrogen at various energy shares 11 (15) when air-to-fuel ratio is fixed. The results for NOx reduction correlate closely with 12 experimental work in literature and follow a similar trend for NOx reduction in spark 13 14 ignition engines to that reported by Ji et al. (19).

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16 **5.Conclusions**

In this research, a 4-cylinder gasoline engine was optimized for hydrogen injection as the secondary fuel using AVL software. This study has addressed the power loss in hydrogen/gasoline dual fueled engines with a novel and innovative approach. The effect of water injection, SOC modification and hydrogen injection at different energy shares on the performance of a hydrogen/gasoline dual fueled engine, has been investigated. The hydrogen has been injected into the engine at different energy shares. The main results drawn from this study may be summarized as follows: Optimized co-injection of water with start of combustion (SOC) modification in
 various hydrogen energy shares achieves good compensation of the power drop
 due to hydrogen injection as indicated by BMEP.

- Injection of hydrogen without any modification results in a reduction in engine
 brake thermal efficiency between 0.3% and 1.2% for various hydrogen energy
 shares. However, by injection of water and modification of SOC with optimum
 values, the engine brake thermal efficiency is successfully increased due to the
 increase of heat release rate even above the original single fueled engine.
- 9 The peak of net rate of heat release is increased by optimum co-injection of water
 10 and hydrogen compared to hydrogen/gasoline dual fueling mode without water
 11 injection and SOC modification.
- The engine equivalent BSFC considerably increases by injection of hydrogen at
 various energy shares; however, with optimized co-injection of water and
 hydrogen, the engine equivalent BSFC decreases to between 1.23% and 3%
 compared to the original condition.
- By water injection into the engine, the total temperature of the in-cylinder gas
 mixture decreases, indicating that the engine NOx rate has dropped below the rate
 of single fuel and dual fueled engines without modification.
- Optimized simultaneous injection of water and hydrogen into the engine results
 in a CO reduction rate of about 25% compared to the single and dual fueled mode;
 however, the HC production rate increases relative to other fueling modes at
 various hydrogen energy shares caused by the moderate increase of unburnt zones
 in the engine combustion chamber by water injection.
- The results of this work have demonstrated the benefits of adding water to
 hydrogen/gasoline dual fuel engine and SOC tuning for compensating the power

loss caused by hydrogen injection at various energy shares as well as the NOx
 reduction. It can be a valuable reference for automotive industry for future testing
 of the proposed solutions in real practice.

- The results of this study confirm the need for further modifications and the
 optimization approach in designing 21st century hydrogen injection mechanisms
 for hydrogen/gasoline dual fueled engines. The study of temperature variation of
 injected water into the engine is suggested for future research. Furthermore, more
 complex combustion model such as fractal can be considered instead of the Vibe
 two-zone model in future works.

Nomenclature		
а	Vibe parameter	
BMEP	Brake mean effective pressure	
BSFC	Brake specific fuel consumption	
BDUR	Burn duration	
C	Cylinder	
CAT	Catalytic converter	
CL	Air cleaner	
cte	Constant parameter	
E	Engine	
ED	Electrical generator	
EV	Electric vehicle	
FCHEV	Fuel cell hybrid electric vehicle	
HEV	Hybrid electric vehicle	
IC engine	Internal combustion engine	
LHV	Lower Heating Value	
m	Vibe shape	
МС	Mechanical connection	
МР	Measuring point	
РСТ	Peak cylinder temperature	
PL	Plenum	
SB	System boundary	
SOC	Start of combustion	
WIR	Water injection ratio	
α	Crank shaft angle	
Subscripts		
ES	Energy share	

1 6.Acknowledgement

2 AVL List GmbH support for proving the simulation tools for University of Salford

3 through their University Partnership Program is greatly appreciated. Special thanks to

4 Dina Motors company for their support during this research.

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